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Phase Transitions in Hexafluophosphate Salts,* K. Vedam, R. Pepinsky, Joseph Lajzerowicz, Y. Okaya and N. Stemple, The Pennsylvania State University.——
$NH_4PF_6 \cdot NH_4F$ is tetragonal at room temperature, and has two low-temperature transitions: at -45°C (= T_{uc}) and at -101°C (= T_{Lc}).[1] Both low-temperature phases are orthorhombic. The dielectric constant $\varepsilon_{[110]}$ exhibits a small anomaly at T_{uc}, and a pronounced anomaly at T_{Lc}. X-ray examination reveals superstructuring along the a and b axes below T_{uc}, and a doubling of the c axis below T_{Lc}. The lowest phase is antiferroelectric. A detailed structural investigation is required to reveal the dielectric character of the intermediate phase.

An order-disorder transition has been observed in KPF_6 at 4°C.[1] A detailed x-ray structure analysis reveals hindered rotation of the $(PF_6)^{-1}$ octahedra. A large thermal anomaly at the transition temperature suggests a "freezing in" of the hindered rotations in the lower phase.

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[1] R. Pepinsky et al., Acta Cryst. 10, 835 (1957).